

Tris(2-butoxyethyl) phosphate  
78-51-3 | DTXSID5021758

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -59.7 °C

Global applicability domain: Inside

Local applicability domain index: 3.58e-01

Confidence level: 4.07e-01

Nearest Neighbors from the Training Set

Image not found

Tris(2-butoxyethyl) phosphate

Measured: -70.0

Predicted: -59.7

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Bis[2-(2-butoxyethoxy)ethyl]  
hexandioate

Measured: -47.0

Predicted: -38.9

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cis-Mevinphos

Measured: 21.0

Predicted: 15.8

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Acetyl tributyl citrate

Measured: -80.0

Predicted: -40.7

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Tetraethyl ethane-1,1,2,2-  
tetracarboxylate

Measured: 77.0

Predicted: 46.2